
Supporting information to:

**Computational Study revealed a “Pull-Push” Radical Transfer
Mechanism of Mmp10-Catalyzed C₅-methylation of Arginine**

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S1. Computational details

The quantum chemical cluster calculations were performed using the density functional B3LYP-D3^{S1} (with the default D3 dispersion correction^{S2} as proposed by Grimme) as implemented in the Gaussian 16 program.^{S3} All geometries were optimized using the 6-31G(d,p) basis sets for the C, N, O, H elements, while the SDD pseudopotential^{S4a} and its corresponding basis sets for Co (**BS1**). On the basis of these optimized geometries, more accurate energies were obtained by performing single-point calculations using the 6-311+G(2d,2p) basis sets for all atoms except Co, for which the revised SDD^{S4} (with *2f* and *1g* polarized functions) was used (**BS2**). To evaluate the sensitivity of the results to the choice of density functional, single-point calculations were carried out using the hybrid meta-GGA functional MN15^{S5} based on the B3LYP-D3 geometries. Both methods gave quite similar barriers and reaction energies.

Analytic frequency calculations were done at the same theory level as the geometry optimizations to obtain the zero-point energies (ZPE) and to confirm the nature of various stationary points. As shown in **Figure 2**, a number of atoms at the boundary of the model were kept frozen during the geometry optimization. This coordinate locking scheme leads to a few small imaginary frequencies, which contribute little to the ZPE and thus can be disregarded.

The solvation effects of the enzyme environment were calculated as single points at the same theory level as the geometry optimizations using the SMD^{S6} solvation model method. The dielectric constant was chosen to be 4, which is commonly used in the modeling of protein surroundings. For comparison, a dielectric constant of 80 (water) was also used, and it gave very similar results (**Figure S5**), with a root-mean-squared deviation (RMSD) of 0.6 kcal/mol.

The principal interacting orbital (PIO) analysis^{S7} was performed using the B3LYP-D3 wavefunctions and the publicly available code on Github, combined with the natural population analysis carried out by the NBO 7.0 package.^{S8}

Basis sets used for geometry optimization (BS1, in Gaussian format).

Co
SDD

C N O H
6-31g(d,p)

Co
SDD

Basis sets used for single single-point calculations (BS2, in Gaussian format).

Co 0
S 3 1.00
20.9080010 0.3980530
13.9062340 -0.6490520
7.3285430 -0.7234530
S 1 1.00
2.1363240 1.0
S 1 1.00
0.8528220 1.0
S 1 1.00
0.1066920 1.0
S 1 1.00
0.0393460 1.0
S 1 1.00
0.0100000 1.0
P 2 1.00
67.0344430 0.0293700
13.2623340 -1.0136260
P 2 1.00
5.6906500 0.2038650
2.2719400 0.8336450
P 1 1.00
0.7889110 1.0
P 1 1.00
0.1183550 1.0
P 1 1.00
0.0305940 1.0
D 4 1.00
36.8405200 0.0380560
11.1736750 0.1889250
3.7975640 0.4410510

1.2392620 0.5656970

D 1 1.00

0.3394000 1.0

D 1 1.00

0.0900000 1.0

F 1 1.00

4.0760000 1.0

F 1 1.00

1.0190000 1.0

G 1 1.00

2. 7110000 1.0

C N O H 6-311+G(2d,2p)

Co

SDD

S2. Tables, Figures, and Schemes

Table S1. Calculated Mulliken spin populations on key atoms of various stationary points.

Entry	Complex	Spin population				
		C1	C2	C3	C4	Co
1	React	1.06	0.00	0.00	0.00	0.00
2	TS1	0.59	0.44	0.00	0.00	0.00
3	Int1	0.00	0.84	0.00	0.00	0.01
4	TS2	0.00	0.61	-0.47	0.00	0.80
5	TS2'	0.00	0.37	0.00	0.52	0.00
6	Int2'	0.00	0.00	0.00	0.96	0.00
7	TS3'	0.00	0.01	-0.46	0.79	0.76
8	Prod	0.00	0.00	0.00	0.00	1.10
9	Prod'	0.00	0.00	0.00	0.00	1.10

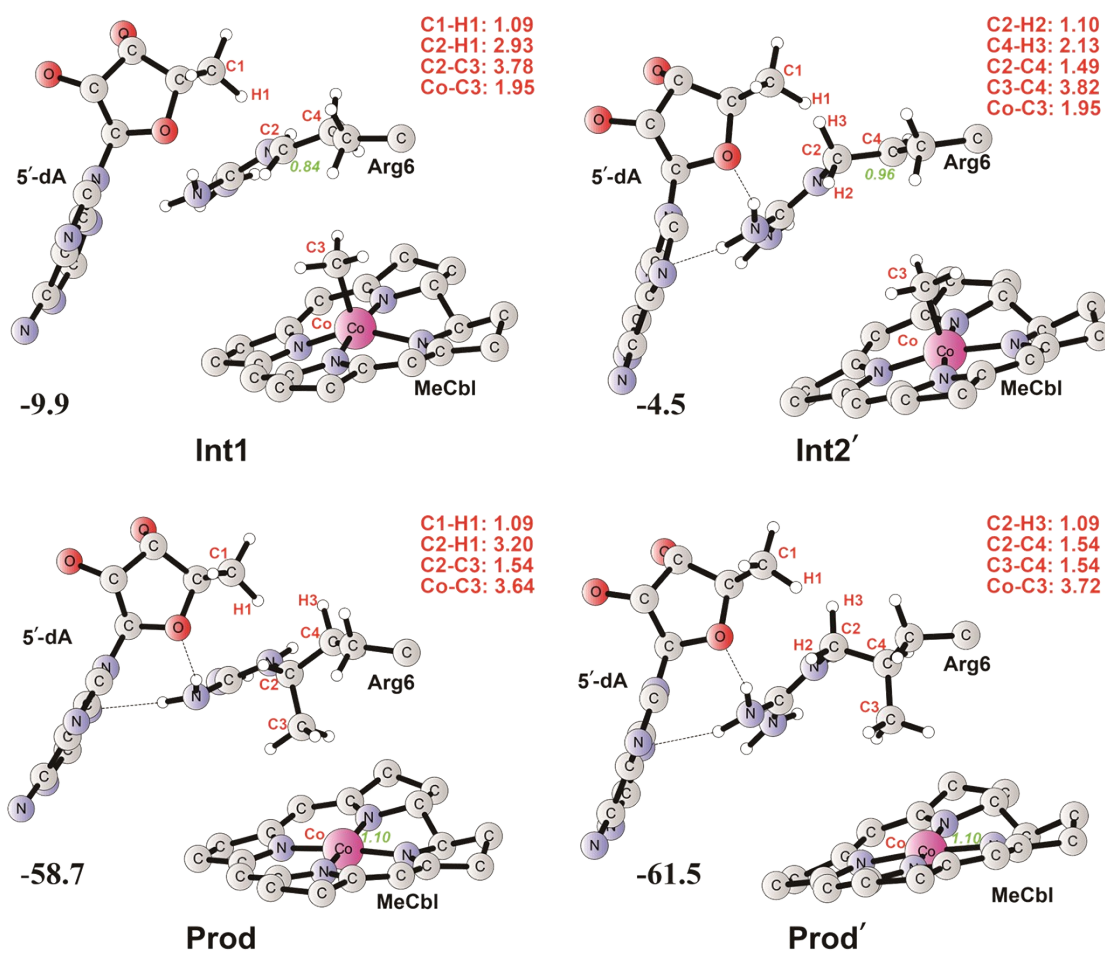


Fig. S1 Optimized structures of intermediates and products.

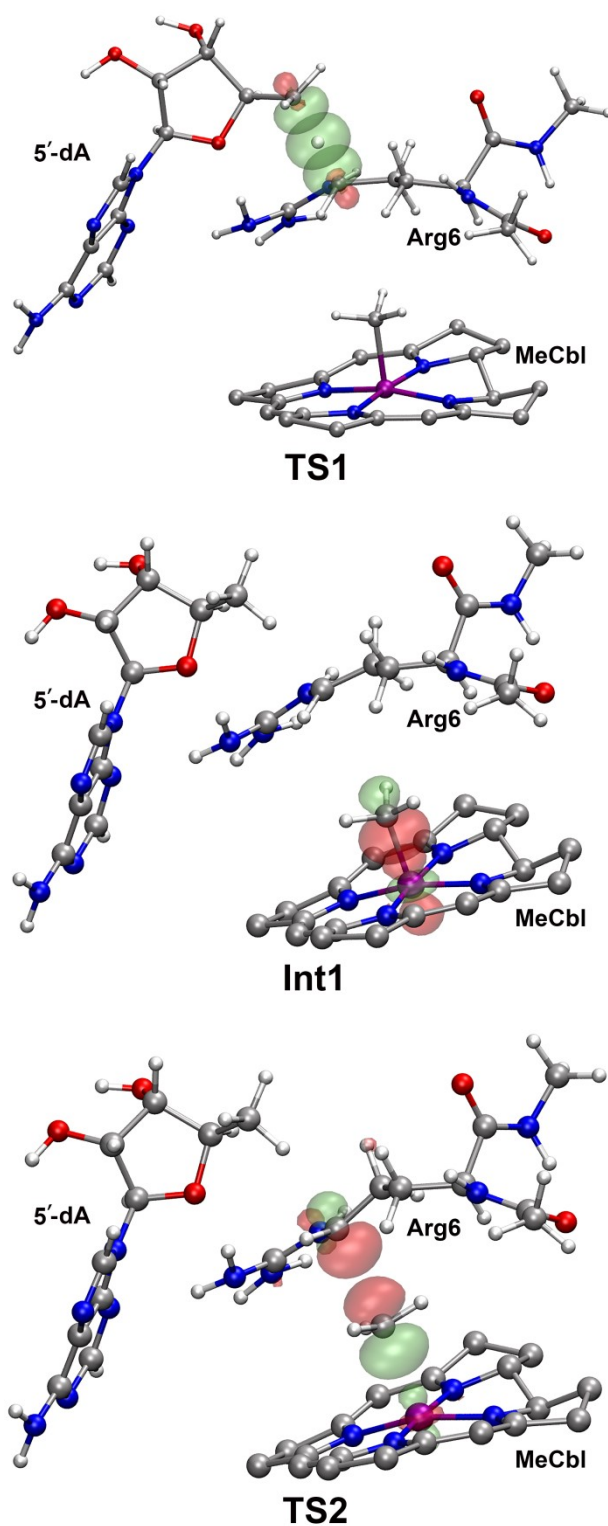


Fig. S2 PISO analysis on **TS1**, **Int1**, and **TS2**. For **TS1**, the two fragments are the transferred hydrogen atom and the rest of the model. For **Int1** and **TS2**, the two fragments are the transferred methyl group (CH₃) and the rest of the model. The α -PISOs are presented as the β -PISOs are very similar. The first α -PISO and β -PISO have an overall contribution of 99.4%, 92.0%, and 91.0%, respectively, for **TS1**, **Int1**, and **TS2**, respectively. These suggested that these orbitals captured most of the interactions.

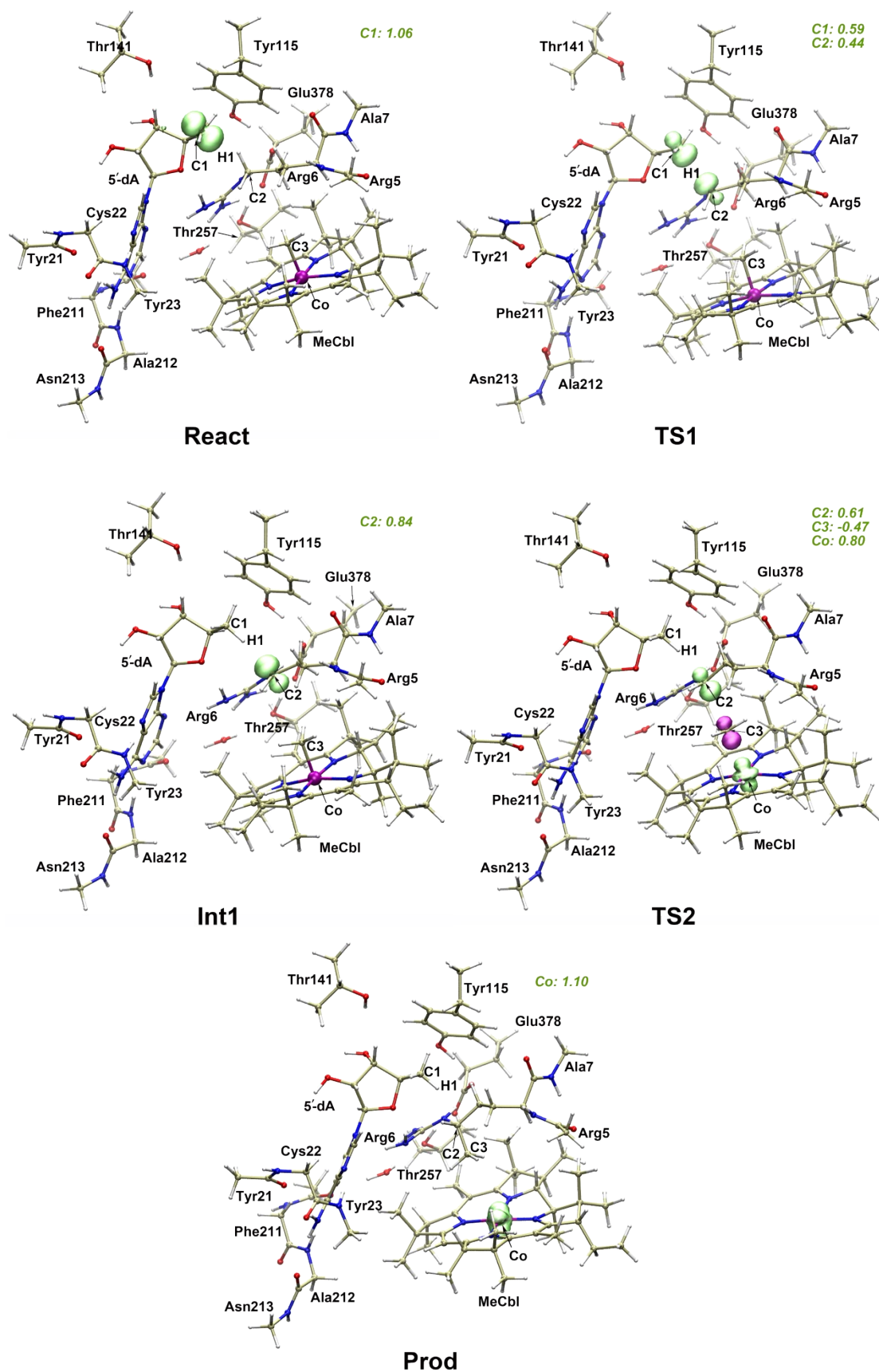


Fig. S3 Plots of Mulliken spin density in various stationary points.

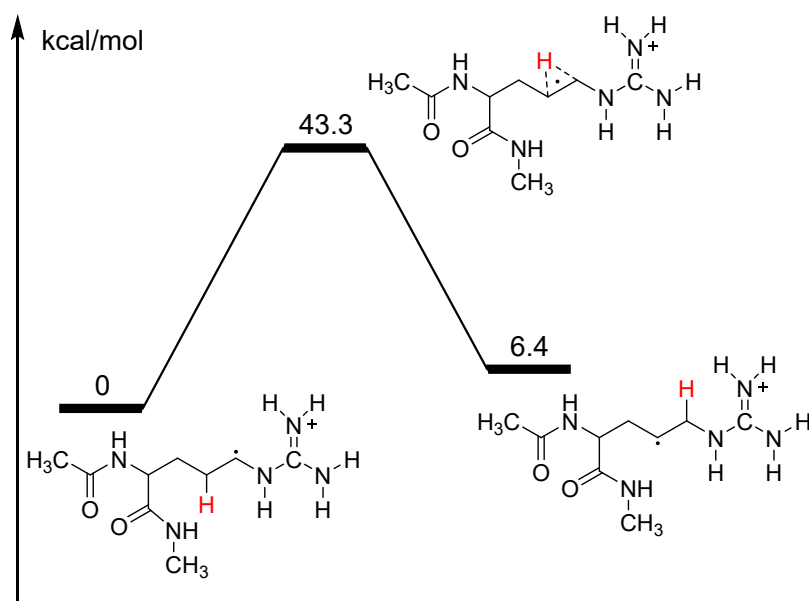


Fig. S4 Energy diagram (in kcal/mol) for 1,2-hydrogen shift step of C₆-centered radical arginine at the B3LYP-D3/6-311+G(2d,2p) level.

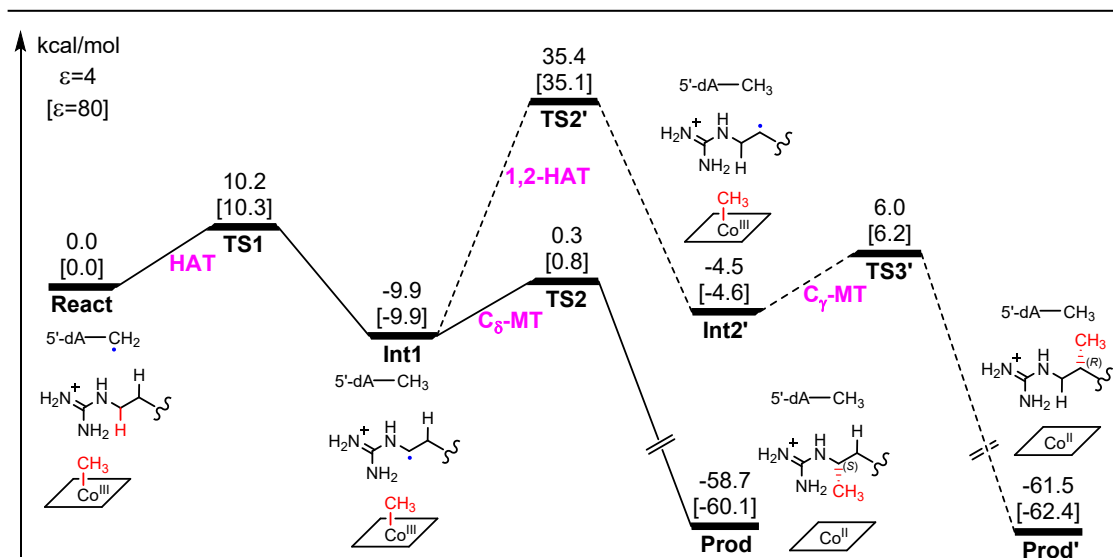
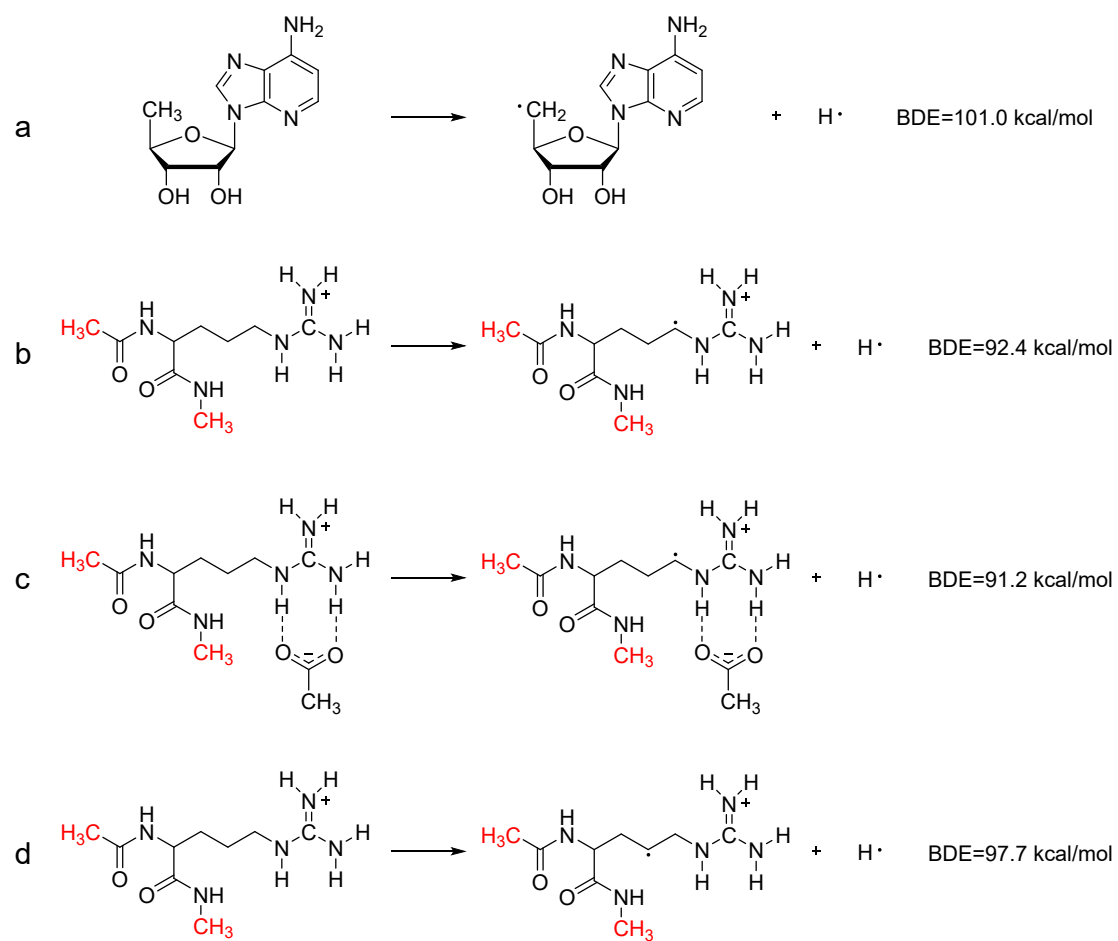
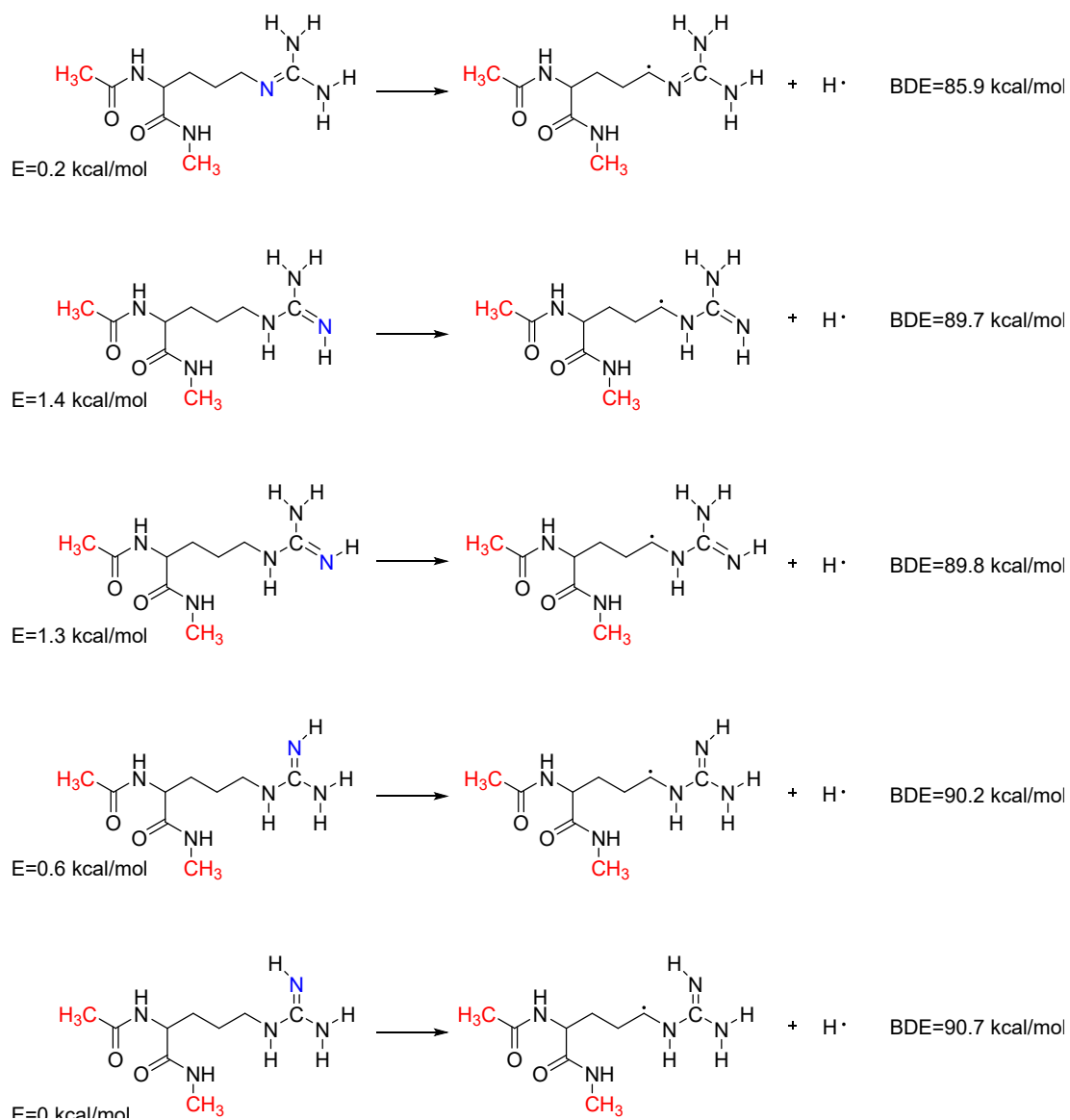


Fig. S5 Energy diagram (in kcal/mol) at the B3LYP-D3 level using two different dielectric constants ($\epsilon=4$ and $\epsilon=80$) to model the solvation effects.



Scheme S1. Bond dissociation energies of 5'-deoxyadenosine (a) and arginine (b, c, and d). All calculations were carried out at the B3LYP-D3/6-311+G(2d,2p) level. The present energies include zero-point energy corrections.



Scheme S2. Bond dissociation energies of arginine in different protonated states. Relative energies of different protonated arginines are shown on the left side. All calculations were carried out at the B3LYP-D3/6-311+G(2d,2p) level. The present energies include zero-point energy corrections.

S3. Energies for all stationary points

Table S2. Calculated energies (in Hartree) for all stationary points.

	optimization	solvation	large basis sets	ZPE
²React^a	-5717.34136	-5717.41484	-5718.99724	2.31022
⁴React	-5717.30652	-5717.37981	-5718.96315	2.30775
²TS1	-5717.32335	-5717.39771	-5718.97691	2.30704
²Int1	-5717.35830	-5717.43155	-5719.01359	2.31059
⁴Int1	-5717.32314	-5717.39612	-5718.97929	2.30771
²TS2	-5717.34259	-5717.41445	-5718.99721	2.30901
²TS2'	-5717.27922	-5717.35321	-5718.93543	2.30531
²Int2'	-5717.34801	-5717.42230	-5719.00365	2.31033
²TS3'	-5717.33126	-5717.40411	-5718.98647	2.30836
²Prod	-5717.43895	-5717.51642	-5719.09252	2.31598
⁴Prod	-5717.38884	-5717.47021	-5719.04231	2.31272
²Prod'	-5717.443577	-5717.52189	-5719.09706	2.31683

^aThe superscript shown in the left indicates the multiplicity.

S5. Cartesian Coordinates of Optimized Structures

React			
C	-14.82269000	30.21609000	19.63219300
C	-14.43410500	28.90462500	19.06747600
O	-13.77564400	29.14331700	17.77164200
C	-13.41425200	28.06640400	19.90171900
O	-13.83073800	26.70563100	19.89436700
C	-12.11353100	28.22298000	19.09921200
O	-11.25445500	27.13980800	19.37187000
C	-12.65789500	28.27353600	17.66106600
N	-11.74362400	28.78148600	16.66143400
C	-10.93289600	29.90306700	16.74158000
N	-10.18243200	30.07831500	15.68266700
C	-10.50403600	29.02618000	14.83587000
C	-10.01717000	28.61652800	13.56256500
N	-8.98716400	29.21884800	12.94510700
N	-10.65622500	27.58283100	12.95548700
C	-11.66349400	26.96173400	13.59504300
N	-12.13809900	27.20445000	14.82547000
C	-11.50686800	28.23763500	15.40406100
Co	-17.67795700	32.29364400	11.49018400
N	-19.01623600	33.61178100	11.45070700
N	-16.35182700	33.67156000	11.27308200
N	-16.53751900	30.79437700	11.08783900
N	-19.12029600	31.13850800	11.73520000
C	-20.41955600	33.11968000	11.35708000
C	-20.71569400	32.79898200	9.87944900
C	-21.25217400	34.33087500	11.91826500
C	-22.69160700	34.41535500	11.39547200
C	-21.29581600	34.31293000	13.45740300
C	-20.33974300	35.54397600	11.50745700
C	-20.66539800	36.28988500	10.17408100
C	-21.41505300	37.59495700	10.46007400
C	-18.96281700	34.91128300	11.52458600
C	-17.74227800	35.65945700	11.62805900
C	-17.90806100	37.14455300	11.88590300
C	-16.51953200	35.03986800	11.49523400
C	-15.16197800	35.76056500	11.44261300
C	-15.09154300	36.57128900	10.12682200
C	-14.82057800	36.65159600	12.65656900
C	-14.17383000	34.56164500	11.44788800
C	-12.96797000	34.68699800	10.53900900
C	-15.04139900	33.36582100	11.17704200

C	-14.51052300	32.10371800	10.94989000
C	-15.21234900	30.90354700	10.88384300
C	-14.52987200	29.55093600	10.72830100
C	-13.49168200	29.51627500	9.59696100
C	-13.83246200	29.22165600	12.07059900
C	-15.74981700	28.59538900	10.54430000
C	-15.98497800	28.06001200	9.10498600
C	-16.91191300	29.44878200	11.04971400
C	-18.13936700	28.95305100	11.42666400
C	-18.34539500	27.45449200	11.46696100
C	-19.22708800	29.83793300	11.77861600
C	-20.62135200	29.42631700	12.26939800
C	-20.51501400	29.01366200	13.75129500
C	-21.28304400	28.34595500	11.42204400
C	-21.43088300	30.75299000	12.08545100
C	-22.62114800	30.91728400	13.02962600
C	-20.34910300	31.82296200	12.19136000
C	-17.29917500	32.26144700	13.40197400
C	-19.36770900	32.90910600	17.07434100
C	-18.09706900	32.05491900	17.11841600
C	-18.32740500	30.62038600	16.65095400
C	-17.04791500	29.79009600	16.77179100
N	-17.21447100	28.51288500	16.09172500
C	-16.29078900	27.90214200	15.34324600
N	-15.01765000	28.37696400	15.29343600
N	-16.63714900	26.84871300	14.61293400
C	-5.10613400	28.26183200	16.21419300
C	-6.21179200	29.33529600	16.14433900
O	-7.18834900	29.17016800	15.41100800
N	-6.09131600	30.44995100	16.92722900
C	-7.09804400	31.52495400	16.91200100
C	-7.10855800	32.29923500	15.56745500
O	-6.08850400	32.82214000	15.13739600
N	-8.32594700	32.38014200	14.96017100
C	-8.47604800	33.01601500	13.65200000
C	-17.87842300	30.28504100	24.18704100
C	-17.50476700	30.63336400	22.72019900
C	-17.76884200	29.54335200	21.70080300
C	-17.00287000	28.36316900	21.71728100
C	-18.72893900	29.68703500	20.69241600
C	-17.17791600	27.37208900	20.75528000
C	-18.92648800	28.69243100	19.72990400
C	-18.14380400	27.52836600	19.74759500
O	-18.27114900	26.54228400	18.82666500

C	-13.71991800	25.19936600	24.47683000
C	-13.12273200	26.35559600	23.66402700
O	-14.11766400	27.07747300	22.92774300
C	-12.01285700	25.86057000	22.73062000
C	-13.22503500	22.26107200	11.26005000
C	-12.27837600	23.43648000	11.45451900
O	-12.72465700	24.54983500	11.76297600
N	-10.95009000	23.18897500	11.30998200
C	-9.92401700	24.22799900	11.39697800
C	-9.79696600	24.98658400	10.06904400
O	-9.54051900	24.37874500	9.03280000
N	-10.00145400	26.32715100	10.13869900
C	-9.78101600	27.15299200	8.96402200
C	-8.40366200	27.79115700	8.99815900
O	-7.99173800	28.39512600	9.99005500
N	-7.72051700	27.64945100	7.83974300
C	-6.37599100	28.13600200	7.66100000
C	-19.32865900	22.74722800	11.65441700
C	-19.54801700	24.19738400	12.05639900
O	-18.42382900	24.60024000	12.84792100
C	-20.88386900	24.37859400	12.77858000
C	-23.26170800	24.64413100	16.90937600
C	-22.27886500	25.80843300	16.71756500
C	-20.87238600	25.27474900	16.37957200
C	-19.88838600	26.33906400	15.91446900
O	-19.67584400	27.33729200	16.66942400
O	-19.30987500	26.18870100	14.79400100
O	-15.51324000	25.55932500	12.36573000
H	-17.71835700	32.06112500	18.14783600
H	-17.34459800	32.52735900	16.47440800
H	-18.64897300	30.62371600	15.60449400
H	-19.12507400	30.14178400	17.22673000
H	-16.81444500	29.64444600	17.83208000
H	-16.21563900	30.33586400	16.31554500
H	-18.14283000	28.05942400	16.20153900
H	-17.63471500	26.59833700	14.59211600
H	-15.99620400	26.39772400	13.95612600
H	-14.68332500	28.86003600	16.12525500
H	-14.31482500	27.75870500	14.89615100
H	-19.86899500	32.79471800	16.10715900
H	-4.54703700	28.29157600	15.27389000
H	-8.07499700	31.08347000	17.12450300
H	-7.76790900	32.59841300	12.92660300
H	-16.43125400	30.86575100	22.69157500

H	-18.01698400	31.55185600	22.41263800
H	-16.24030600	28.22324400	22.48063300
H	-19.32541200	30.59301300	20.64020400
H	-16.56886100	26.47375600	20.75106500
H	-19.69516400	28.80090300	18.96973700
H	-18.91017700	26.82212900	18.13222600
H	-17.87696600	29.20155600	24.34088900
H	-12.74529600	21.28336300	11.34036200
H	-10.16562200	24.88897800	12.23113700
H	-9.93506700	26.52585400	8.08408300
H	-6.11221700	28.72180400	8.54263800
H	-19.56781200	24.82083700	11.14683800
H	-21.01019300	25.39988700	13.14420000
H	-21.70807900	24.13902500	12.09913600
H	-20.94743900	23.70266100	13.63753200
H	-18.77128900	25.04054000	13.65212700
H	-20.19843200	22.34017400	11.12709300
H	-22.21637600	26.43015300	17.61661300
H	-22.63031700	26.46485500	15.91047700
H	-20.93630900	24.50030400	15.61313900
H	-20.44594000	24.81017500	17.27855700
H	-22.81831000	23.88124200	17.56131400
H	-15.68545700	30.28626700	20.28207600
H	-14.18365900	31.07699500	19.46994900
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H	-10.95689500	30.55789600	17.60086900
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H	-12.13872200	26.15663900	13.04147700
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H	-20.53499700	33.67211700	9.25108800
H	-20.05761300	31.99739300	9.53363800
H	-23.19834600	35.28117800	11.83173600
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H	-23.25995000	33.52803000	11.68623200
H	-20.29845200	34.25127800	13.90036200
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H	-18.31109700	37.32343600	12.89017700
H	-18.60503500	37.59801200	11.17830800
H	-14.12065800	37.06264500	10.02238300
H	-15.24740300	35.92827600	9.25562700
H	-15.85851100	37.34697700	10.10329500
H	-15.31797300	37.62113200	12.64756400
H	-13.74266000	36.84758300	12.65622200
H	-13.80823400	34.43307100	12.47779500
H	-13.24701200	34.68463600	9.48266200
H	-12.26573000	33.86382200	10.69822900
H	-13.43381100	32.03738500	10.86406400
H	-13.07359400	28.50851000	9.50763200
H	-12.65991900	30.19373000	9.81288700
H	-13.91722100	29.80098900	8.63164000
H	-13.40339600	28.21772500	12.01798000
H	-14.53935200	29.24901300	12.90461000
H	-13.02257300	29.92673500	12.28336900
H	-15.61800700	27.72223200	11.18998700
H	-16.13795900	28.87450700	8.38971400
H	-16.87064100	27.42140800	9.08580800
H	-18.87229500	27.13957800	12.36628000
H	-18.91955100	27.09654100	10.60605500
H	-17.40189400	26.91523500	11.47816000
H	-21.48565900	28.67869500	14.12808400
H	-19.81529900	28.19283700	13.90059800
H	-20.18612900	29.85147500	14.37034400
H	-22.36397800	28.35789800	11.60207500
H	-20.93878800	27.34013300	11.66079800
H	-21.80597400	30.74546600	11.05595400
H	-23.27580500	30.04160600	12.98698300
H	-23.22561200	31.78541600	12.75811500
H	-17.82816300	33.09428100	13.87294000
H	-17.63379700	31.30503400	13.80445500
H	-16.21937900	32.36278900	13.53388300
H	-14.25321800	24.51102400	23.80990900
H	-12.70016300	27.09604700	24.35443200
H	-14.34467600	26.57149400	22.13237200
H	-11.61804800	26.67608400	22.11770600
H	-11.18497300	25.42105900	23.29574400
H	-12.40000300	25.07993800	22.06181200
H	-14.71054000	25.04653500	12.15998400

H	-16.28501500	24.96563900	12.35049900
H	-21.98165900	38.01288100	9.62785400
H	-21.74813200	35.22967900	13.84117900
H	-15.13040700	27.46326100	8.77824300
H	-21.12493200	28.52127500	10.35286100
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H	-24.21108200	24.92071000	17.36831600
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H	-17.11634900	30.70396800	24.84478300
H	-14.41281900	25.52108300	25.25446300
H	-12.92057200	24.63109800	24.96636200
H	-4.40180800	28.34688100	17.04160600
H	-6.83965600	32.23216700	17.70273400
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H	-9.02771500	31.69217000	15.23397500
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H	-9.49310200	32.83115000	13.29852000
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H	-22.11728900	31.91378000	19.84862800
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H	-23.18855100	31.04875300	18.74201800

TS1

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Int1

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TS2

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TS2'

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H	-23.22562800	31.79497300	12.72295800
H	-17.68080400	33.23853200	13.83676900
H	-17.83883500	31.44518300	13.89351700
H	-16.24448000	32.18812400	13.56383400
H	-14.24024600	24.47481300	23.83849100
H	-12.73648400	27.10864900	24.28684300
H	-14.44525100	26.54881900	22.12422400
H	-11.73276400	26.67943100	22.01964700
H	-11.24552300	25.43089000	23.18440600
H	-12.50439000	25.07902000	21.99792800
H	-14.66547400	25.05329800	12.11278100
H	-16.24049300	24.94506400	12.28711700
H	-21.98162100	38.01289100	9.62784600

H	-21.74702800	35.23315400	13.82665300
H	-15.13123200	27.46340200	8.77593200
H	-21.12857300	28.50861100	10.35019900
H	-23.47469000	24.12263800	15.96995100
H	-24.21112900	24.92062600	17.36824800
H	-18.86361600	30.66983200	24.46207900
H	-17.11638100	30.70401600	24.84484600
H	-14.41290800	25.52110100	25.25443900
H	-12.89349500	24.67332500	24.96824000
H	-4.40180700	28.34688200	17.04161100
H	-6.83988300	32.23317000	17.70194600
H	-8.30674300	34.09231300	13.68538800
H	-8.65947100	28.81930700	12.09924500
H	-9.03561100	31.70062800	15.23976400
H	-5.19635600	30.64938500	17.35108500
H	-5.66479600	27.30739300	7.56717300
H	-6.28902300	28.77002900	6.77864600
H	-8.10685900	27.03870600	7.13692800
H	-10.17260300	26.77891900	11.03932100
H	-10.67642700	22.31833300	10.87827400
H	-8.96536400	23.74343700	11.59582500
H	-19.12531300	22.14983100	12.54767400
H	-18.47643300	22.68892000	10.97726700
H	-13.71801900	22.34358500	10.28661900
H	-5.60204700	27.29030000	16.26319800
H	-22.30453400	31.05761600	14.03784500
H	-21.87637500	32.43954900	16.94706300
H	-18.22797200	34.52794800	17.76273700
H	-15.03829200	36.04429300	13.68605700
H	-9.49273300	32.83115000	13.29703300
H	-13.97954400	22.37745500	12.03789000
H	-12.40338700	35.60183500	10.74256800
H	-10.51917600	27.96390600	8.95198000
H	-20.18369500	32.10031400	13.22270600
C	-19.30570000	36.72563700	17.01985800
C	-19.84425400	35.32188500	16.78043400
O	-20.94467000	35.10061900	16.28125700
N	-18.99896300	34.31215100	17.14600600
C	-20.31117700	32.52592100	18.22245700
O	-19.88236800	32.55121300	19.37143900
N	-21.58029000	32.16637500	17.87401800
C	-22.61787900	31.96693200	18.88110500
H	-18.21797700	36.77805900	16.91859500
H	-19.77649500	37.41054500	16.31395100

H	-19.57292300	37.05069500	18.03145100
H	-22.12372700	31.92087300	19.85253700
H	-23.31547700	32.81221000	18.88905900
H	-23.18866900	31.04880200	18.74198300

Int2'

C	-14.70499900	30.30612600	19.71666700
C	-14.42724000	28.94712300	19.10409500
O	-13.81000300	29.16585800	17.78487900
C	-13.43713000	28.06722200	19.89442900
O	-13.89322000	26.71798200	19.87563900
C	-12.14184000	28.19464700	19.07677800
O	-11.31452400	27.08006800	19.31897900
C	-12.70453700	28.28485500	17.64665800
N	-11.79042000	28.79769500	16.64779300
C	-10.97307100	29.91392000	16.73598200
N	-10.20855000	30.08271500	15.68568500
C	-10.52636800	29.03028800	14.83738500
C	-10.02866100	28.61529700	13.56997900
N	-8.99178400	29.21321300	12.95966900
N	-10.66444700	27.58125500	12.95985800
C	-11.68100000	26.96621800	13.59015000
N	-12.16959100	27.21632500	14.81358300
C	-11.54026400	28.24870500	15.39587600
Co	-17.67350000	32.29458500	11.51241100
N	-19.01063400	33.61270600	11.46349500
N	-16.34314300	33.67036800	11.30213400
N	-16.53250600	30.79378000	11.10676800
N	-19.11464100	31.13908100	11.74282800
C	-20.41343900	33.12035600	11.36773400
C	-20.70824500	32.80049900	9.88960500
C	-21.24589500	34.33181500	11.92830200
C	-22.68626200	34.41428800	11.40812500
C	-21.28634900	34.31537900	13.46787100
C	-20.33493900	35.54554900	11.51418200
C	-20.66237000	36.28941200	10.17894100
C	-21.41509800	37.59494800	10.46010800
C	-18.95700300	34.91230400	11.53542600
C	-17.73573100	35.65931900	11.64419200
C	-17.90370200	37.14464000	11.90017400
C	-16.51186800	35.03926000	11.51811200
C	-15.15397200	35.76039600	11.46843800
C	-15.08393200	36.58197200	10.15938200
C	-14.81456700	36.64178300	12.68998800
C	-14.16329900	34.56224800	11.46423000
C	-12.96801800	34.68698000	10.53905200
C	-15.03289900	33.36452100	11.20507900
C	-14.50349700	32.10174900	10.97773600
C	-15.20743200	30.90304300	10.90292500

C	-14.52702800	29.55148500	10.72838500
C	-13.49736100	29.52939400	9.58885200
C	-13.81972000	29.20737200	12.06126800
C	-15.74822500	28.59735600	10.54279600
C	-15.98502200	28.06000900	9.10504700
C	-16.90968500	29.44968800	11.04945700
C	-18.14060300	28.95334300	11.41075700
C	-18.35344100	27.45504600	11.42587700
C	-19.22458400	29.83883400	11.77118900
C	-20.61488400	29.42610400	12.26737100
C	-20.48206800	29.01337300	13.74764900
C	-21.28297300	28.34598200	11.42195900
C	-21.42554600	30.75339700	12.09659100
C	-22.60638400	30.91323600	13.05327200
C	-20.34289100	31.82268200	12.20127200
C	-17.31326700	32.29968600	13.43139200
C	-19.38679900	32.90953000	17.03202000
C	-18.11753000	32.05323500	17.09785700
C	-18.30559700	30.62649100	16.71966200
C	-17.10765800	29.73535700	16.78548300
N	-17.28625200	28.55130900	15.95803800
C	-16.33040700	27.94420700	15.24844400
N	-15.04602400	28.38547800	15.29001600
N	-16.66220700	26.93411500	14.45370000
C	-5.10612900	28.26182600	16.21418800
C	-6.21515300	29.33237200	16.14952000
O	-7.19746300	29.16263000	15.42485800
N	-6.09037800	30.45070700	16.92664400
C	-7.09802800	31.52496600	16.91200800
C	-7.10994100	32.29776800	15.56707300
O	-6.08966500	32.81856100	15.13480400
N	-8.32739300	32.37950300	14.96007300
C	-8.47617900	33.01599100	13.65201800
C	-17.87835300	30.28495700	24.18701500
C	-17.49450500	30.64717000	22.72666700
C	-17.78714900	29.58718600	21.68460500
C	-17.06907800	28.37761800	21.68501000
C	-18.72692600	29.79104400	20.66808300
C	-17.27448600	27.41309800	20.70179000
C	-18.95265300	28.82639100	19.68233900
C	-18.22129800	27.62915000	19.68736100
O	-18.37629200	26.66808900	18.74366500
C	-13.71975700	25.19931400	24.47692700
C	-13.14811700	26.35582800	23.64519000

O	-14.16118400	27.06204200	22.91731300
C	-12.04600800	25.86542100	22.70041700
C	-13.22503500	22.26100600	11.26001100
C	-12.27772600	23.43620100	11.45010400
O	-12.72356600	24.55260000	11.74928400
N	-10.94939400	23.18786800	11.31177900
C	-9.92397100	24.22797500	11.39696100
C	-9.79867700	24.98612200	10.06839500
O	-9.54284300	24.37811400	9.03221400
N	-10.00325600	26.32666900	10.13809200
C	-9.78103100	27.15301300	8.96402000
C	-8.40247500	27.78871900	8.99951600
O	-7.98861500	28.38779700	9.99345900
N	-7.72078300	27.65033400	7.83976100
C	-6.37599200	28.13602400	7.66102100
C	-19.32865400	22.74719300	11.65441500
C	-19.54410100	24.19859700	12.05348200
O	-18.41431700	24.60233200	12.83677800
C	-20.87695000	24.38438600	12.78022700
C	-23.26172200	24.64425700	16.90940100
C	-22.29975500	25.82095900	16.68457600
C	-20.87862300	25.30899200	16.37658100
C	-19.91842900	26.37685000	15.87167100
O	-19.76208900	27.43021600	16.56542200
O	-19.30073800	26.17611500	14.78192300
O	-15.48986700	25.55534400	12.30348200
H	-17.73203200	32.12571900	18.13110600
H	-17.35760700	32.50833600	16.44399000
H	-19.29112300	30.16915400	16.71903600
H	-16.93305200	29.44381700	17.83481100
H	-15.29920900	30.91453600	19.02954200
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H	-18.22077000	28.10435000	16.02910300
H	-17.65028100	26.65390400	14.44397600
H	-15.99871500	26.46343800	13.83417800
H	-14.74214400	28.85370600	16.14134800
H	-14.33366800	27.76887600	14.90674400
H	-19.88684600	32.77628400	16.06737700
H	-4.54737700	28.29686200	15.27380500
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H	-7.76723400	32.59819700	12.92761500
H	-16.41485200	30.85126100	22.70626500
H	-17.97878400	31.58646000	22.43707500
H	-16.32054800	28.19219200	22.45315200

H	-19.28465500	30.72195000	20.62669000
H	-16.70162400	26.49139000	20.68609200
H	-19.69438500	28.99369300	18.90606700
H	-19.01009700	26.97397700	18.05523200
H	-17.87350400	29.20055600	24.33348300
H	-12.74546800	21.28326100	11.34117000
H	-10.16517000	24.88951900	12.23093100
H	-9.93556200	26.52658500	8.08361500
H	-6.11183400	28.72165100	8.54266300
H	-19.56626800	24.81955500	11.14243300
H	-21.00441400	25.40887900	13.13580500
H	-21.70334800	24.13585300	12.10670400
H	-20.93557900	23.71724100	13.64640600
H	-18.75667700	25.01567900	13.65696900
H	-20.19881600	22.34002900	11.12785000
H	-22.25856100	26.47471700	17.56183700
H	-22.65856200	26.44192500	15.85311800
H	-20.91646800	24.50064700	15.64379500
H	-20.44451500	24.89474700	17.29640400
H	-22.80300400	23.90512600	17.57789500
H	-15.27554600	30.18221600	20.63910300
H	-13.77254500	30.83828000	19.93201900
H	-15.35121200	28.37844000	18.96685100
H	-13.32126700	28.40798900	20.92957900
H	-13.10378200	26.15910100	19.95111700
H	-11.64320500	29.14090500	19.33124400
H	-10.53429300	27.12430900	18.75102200
H	-13.01333500	27.28802900	17.30858800
H	-11.00514000	30.57086600	17.59344700
H	-8.32021000	29.68480800	13.55647700
H	-12.15236100	26.16029600	13.03467100
H	-21.74273400	32.48306400	9.74403700
H	-20.52706800	33.67381800	9.26169800
H	-20.04994500	31.99907800	9.54405000
H	-23.19346000	35.27965300	11.84484000
H	-22.75594700	34.50204400	10.32313100
H	-23.25281200	33.52610700	11.70011600
H	-20.28764000	34.25280100	13.90798600
H	-21.87638500	33.48302100	13.85744500
H	-20.38218200	36.29521800	12.31069700
H	-21.25536400	35.64612900	9.52695900
H	-19.73879100	36.49436000	9.62606500
H	-20.73430300	38.37241800	10.82348700
H	-22.15234800	37.43315700	11.25544700

H	-16.97733000	37.70173000	11.83465300
H	-18.31857900	37.32325900	12.89967000
H	-18.59252400	37.59845900	11.18459200
H	-14.11230100	37.07239900	10.05775400
H	-15.24202400	35.94648500	9.28316600
H	-15.84913600	37.35935700	10.14247500
H	-15.32194700	37.60619300	12.69414600
H	-13.73858900	36.84818300	12.68651200
H	-13.78393300	34.43612300	12.48927900
H	-13.26046800	34.68495300	9.48647000
H	-12.26519700	33.86262200	10.68937700
H	-13.42694000	32.03447400	10.89019200
H	-13.07841500	28.52324900	9.48636500
H	-12.66514600	30.20635400	9.80458200
H	-13.93107000	29.82251000	8.62968500
H	-13.39453200	28.20276100	11.99516800
H	-14.52030600	29.22941400	12.90064900
H	-13.00595400	29.90766200	12.27502900
H	-15.61766900	27.72398100	11.18846100
H	-16.13910400	28.87310500	8.38848700
H	-16.86994900	27.42063900	9.08688100
H	-18.88511300	27.12742200	12.31753600
H	-18.92643400	27.11431500	10.55710300
H	-17.41270700	26.91065500	11.43270900
H	-21.45155900	28.71455600	14.15584400
H	-19.81020600	28.16628600	13.87075100
H	-20.09394000	29.83351400	14.36019500
H	-22.36276300	28.35853800	11.60752000
H	-20.93848000	27.33968500	11.65677200
H	-21.81019100	30.75177400	11.07054000
H	-23.26160600	30.03779900	13.01369200
H	-23.21338800	31.78311000	12.79277300
H	-17.63985900	33.26372100	13.83103500
H	-17.84437000	31.47679600	13.91540400
H	-16.23460800	32.17282700	13.55569600
H	-14.24648400	24.49365300	23.82297600
H	-12.72386900	27.10577800	24.32439900
H	-14.37564500	26.56269200	22.11415600
H	-11.66365400	26.68055500	22.07923000
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H	-12.43527000	25.07976000	22.03883500
H	-14.67525900	25.05416400	12.11357000
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H	-21.73835900	35.23220800	13.85190200
H	-15.13061000	27.46317400	8.77793200
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H	-23.47649900	24.13114800	15.96546500
H	-24.21109700	24.92060700	17.36830400
H	-18.86497500	30.66235000	24.46687400
H	-17.11640700	30.70406500	24.84485400
H	-14.41295200	25.52111900	25.25436500
H	-12.90742000	24.65164200	24.96819500
H	-4.40180700	28.34688000	17.04161000
H	-6.83985800	32.23263900	17.70240400
H	-8.30675700	34.09232200	13.68538700
H	-8.66371500	28.83416300	12.07291700
H	-9.03331200	31.69732900	15.23710900
H	-5.19682600	30.64878000	17.35112000
H	-5.66427100	27.30784300	7.56736400
H	-6.28902100	28.77002600	6.77864500
H	-8.10446800	27.03359500	7.13952200
H	-10.17304800	26.77972500	11.03887000
H	-10.67604100	22.31823800	10.87788800
H	-8.96556700	23.74340100	11.59686300
H	-19.13163700	22.13934800	12.54197100
H	-18.47642000	22.68895300	10.97728900
H	-13.71836600	22.34316300	10.28674600
H	-5.60207300	27.29030900	16.26339400
H	-22.27490300	31.03361800	14.08890600
H	-21.89733500	32.43946700	16.93573200
H	-18.21521000	34.52155300	17.73489900
H	-15.05591600	36.12616000	13.62499000
H	-9.49282000	32.83118500	13.29730400
H	-13.97955200	22.37747800	12.03790000
H	-12.41475800	35.60967100	10.73875300
H	-10.52062900	27.96263100	8.95242700
H	-20.17572200	32.09406500	13.24883200
C	-19.30577800	36.72581900	17.01986000
C	-19.84728600	35.32341800	16.78452000
O	-20.95753300	35.10304500	16.30767600
N	-18.99414400	34.31118100	17.12624600
C	-20.32596700	32.53970000	18.20275200
O	-19.89575000	32.57141600	19.35177100
N	-21.59303900	32.17324600	17.86205400
C	-22.61794000	31.96699200	18.88105200
H	-18.21819800	36.77702300	16.91727400
H	-19.77642600	37.41047900	16.31397800

H	-19.57198700	37.05320500	18.03100300
H	-22.11200000	31.91580200	19.84582000
H	-23.31660300	32.81113600	18.90223400
H	-23.18860000	31.04874600	18.74201700

TS3'

C	-14.80147800	30.31738800	19.57566300
C	-14.50132700	28.94799500	18.99623500
O	-13.84105800	29.14427200	17.69320700
C	-13.53091600	28.09216300	19.83714700
O	-13.95735800	26.73397700	19.81211300
C	-12.20538400	28.23753300	19.07129400
O	-11.36170500	27.14875100	19.36841000
C	-12.71317100	28.28229200	17.61968300
N	-11.77572000	28.78521500	16.64009900
C	-10.97428300	29.91345200	16.72313900
N	-10.20398400	30.08078100	15.67704800
C	-10.50192800	29.01607800	14.83669100
C	-9.99513900	28.59894400	13.57346600
N	-8.96894100	29.20908900	12.95784400
N	-10.61428100	27.55079800	12.97098300
C	-11.62329100	26.92592100	13.60301100
N	-12.12047800	27.17937400	14.82186400
C	-11.50904700	28.22683800	15.39594200
Co	-17.56403800	32.27540300	11.63635700
N	-18.86183700	33.64967100	11.50487000
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H	-23.18858600	31.04875300	18.74200700

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